Support information

Study of Surface Thermodynamic Properties of Some Boron Compounds by Inverse Gas Chromatography at Infinite Dilution

Table S1. Values of ($\Delta G_a^{sp}(T)$) (in kJ/mol) of the various polar solvents adsorbed on BPO_4 material against the temperature by using the various models and IGC

ΔG_a^{sp} (T) (in kJ/mol)			Kiselev		
T(K)	**CH_2Cl_2**	**$CHCl_3$**	**THF**	**Ethyl acetate**	**Acetone**
303.15	3.454	1.206	0.157	1.103	4.497
308.15	3.360	1.484	0.270	1.095	4.434
313.15	3.267	1.769	0.382	1.085	4.369
318.15	3.175	2.062	0.494	1.076	4.304
323.15	3.085	2.367	0.607	1.067	4.239
328.15	2.996	2.682	0.719	1.057	4.173

ΔG_a^{sp} (T) (in kJ/mol)			Cylindrical		
T(K)	**CH_2Cl_2**	**$CHCl_3$**	**THF**	**Ethyl acetate**	**Acetone**
303.15	7.106	5.924	-0.925	1.278	2.244
308.15	6.881	5.959	-0.786	1.275	2.237
313.15	6.655	5.996	-0.648	1.270	2.229
318.15	6.431	6.039	-0.508	1.266	2.221
323.15	6.208	6.087	-0.369	1.261	2.213
328.15	5.984	6.140	-0.231	1.256	2.204

ΔG_a^{sp} (T) (in kJ/mol)			VDW		
T(K)	**CH_2Cl_2**	**$CHCl_3$**	**THF**	**Ethyl acetate**	**Acetone**
303.15	4.856	4.125	3.004	2.355	5.257
308.15	4.721	4.297	3.042	2.311	5.164

313.15	4.587	4.475	3.080	2.266	5.072
318.15	4.454	4.660	3.118	2.221	4.979
323.15	4.324	4.854	3.156	2.177	4.887
328.15	4.194	5.058	3.194	2.132	4.794

ΔG_a^{sp} (T) (in kJ/mol)			R-K		
T(K)	**CH_2Cl_2**	**$CHCl_3$**	**THF**	**Ethyl acetate**	**Acetone**
303.15	4.922	4.176	3.051	2.385	5.292
308.15	4.785	4.347	3.087	2.339	5.199
313.15	4.649	4.524	3.123	2.293	5.104
318.15	4.515	4.708	3.160	2.248	5.011
323.15	4.381	4.900	3.196	2.201	4.916
328.15	4.250	5.103	3.232	2.155	4.822

ΔG_a^{sp} (T) (in kJ/mol)			Geometric		
T(K)	**CH_2Cl_2**	**$CHCl_3$**	**THF**	**Ethyl acetate**	**Acetone**
303.15	6.048	3.013	0.747	2.364	2.874
308.15	5.842	3.031	0.849	2.354	2.864
313.15	5.637	3.049	0.951	2.343	2.854
318.15	5.431	3.068	1.053	2.332	2.844
323.15	5.226	3.088	1.155	2.320	2.834
328.15	5.022	3.109	1.257	2.308	2.823

ΔG_a^{sp} (T) (in kJ/mol)			Spherical		
T(K)	**CH_2Cl_2**	**$CHCl_3$**	**THF**	**Ethyl acetate**	**Acetone**
303.15	5.681	4.122	2.911	3.209	6.277
308.15	5.538	4.357	2.945	3.127	6.143
313.15	5.396	4.598	2.980	3.045	6.008
318.15	5.256	4.848	3.015	2.964	5.874
323.15	5.117	5.108	3.049	2.883	5.740
328.15	4.980	5.379	3.084	2.803	5.607

ΔG_a^{sp} (T) (in kJ/mol)			Hamieh model		
T(K)	**CH_2Cl_2**	**$CHCl_3$**	**THF**	**Ethyl acetate**	**Acetone**
303.15	1.878	3.895	6.680	6.691	5.644
308.15	1.843	3.850	6.560	6.591	5.519
313.15	1.808	3.805	6.440	6.491	5.394
318.15	1.773	3.760	6.320	6.391	5.269
323.15	1.738	3.715	6.200	6.291	5.144
328.15	1.703	3.670	6.080	6.191	5.019

ΔG_a^{sp} (T) (in kJ/mol)	Boiling point				
T(K)	CH_2Cl_2	$CHCl_3$	THF	Ethyl acetate	Acetone
303.15	3.384	0.805	1.456	0.740	2.180
308.15	3.236	0.835	1.557	0.802	2.221
313.15	3.088	0.865	1.658	0.864	2.262
318.15	2.941	0.897	1.760	0.927	2.304
323.15	2.793	0.927	1.861	0.989	2.346
328.15	2.646	0.957	1.962	1.051	2.387

ΔG_a^{sp} (T) (in kJ/mol)	Vapor pressure				
T(K)	CH_2Cl_2	$CHCl_3$	THF	Ethyl acetate	Acetone
303.15	2.720	1.273	1.257	2.040	1.714
308.15	2.616	1.305	1.350	2.121	1.788
313.15	2.511	1.337	1.443	2.201	1.862
318.15	2.405	1.369	1.537	2.280	1.936
323.15	2.298	1.399	1.630	2.357	2.009
328.15	2.190	1.430	1.723	2.434	2.082

ΔG_a^{sp} (T) (in kJ/mol)	Deformation polarizability				
T(K)	CH_2Cl_2	$CHCl_3$	THF	Ethyl acetate	Acetone
303.15	0.146	3.737	6.060	4.078	8.154
308.15	0.048	3.728	6.098	4.095	8.114
313.15	-0.052	3.719	6.136	4.111	8.073
318.15	-0.151	3.709	6.174	4.127	8.032
323.15	-0.251	3.700	6.212	4.144	7.991
328.15	-0.349	3.691	6.251	4.161	7.951

ΔG_a^{sp} (T) (in kJ/mol)	Topological index				
T(K)	CH_2Cl_2	$CHCl_3$	THF	Ethyl acetate	Acetone
303.15	8.706	7.366	3.796	2.636	6.539
308.15	8.485	7.305	3.865	2.672	6.520
313.15	8.265	7.245	3.935	2.710	6.503
318.15	8.044	7.184	4.005	2.746	6.484
323.15	7.825	7.123	4.075	2.783	6.466
328.15	7.605	7.063	4.146	2.821	6.449

ΔG_a^{sp} (T) (in kJ/mol)	DHvap				
T(K)	CH_2Cl_2	$CHCl_3$	THF	Ethyl acetate	Acetone
303.15	1.038	0.954	0.701	-0.343	0.980
308.15	0.926	0.984	0.815	-0.264	1.040
313.15	0.814	1.014	0.928	-0.185	1.101

318.15	0.702	1.044	1.042	-0.106	1.161
323.15	0.590	1.074	1.156	-0.027	1.221
328.15	0.477	1.102	1.268	0.051	1.281

Table S2. Values of ($\Delta G_a^{sp}(T)$) (in kJ/mol) of the various polar solvents adsorbed on h-BN material against the temperature by using the various models and IGC

ΔG_a^{sp} (T) (in kJ/mol)			**Kiselev**		
T(K)	**CH_2Cl_2**	**$CHCl_3$**	**THF**	**Ethyl acetate**	**Acetone**
303.15	1.881	1.142	-0.490	0.930	3.540
308.15	1.780	1.207	-0.552	0.840	3.347
313.15	1.681	1.278	-0.614	0.752	3.155
318.15	1.583	1.356	-0.675	0.663	2.964
323.15	1.486	1.443	-0.737	0.576	2.773
328.15	1.390	1.539	-0.798	0.488	2.583

ΔG_a^{sp} (T) (in kJ/mol)			**Cylindrical**		
T(K)	**CH_2Cl_2**	**$CHCl_3$**	**THF**	**Ethyl acetate**	**Acetone**
303.15	3.378	4.296	2.591	2.275	4.335
308.15	3.230	4.236	2.438	2.143	4.112
313.15	3.084	4.182	2.286	2.013	3.891
318.15	2.939	4.133	2.134	1.882	3.670
323.15	2.800	4.097	1.987	1.758	3.454
328.15	2.657	4.064	1.835	1.629	3.235

ΔG_a^{sp} (T) (in kJ/mol)			**VDW**		
T(K)	**CH_2Cl_2**	**$CHCl_3$**	**THF**	**Ethyl acetate**	**Acetone**
303.15	3.378	4.296	2.591	2.275	4.335
308.15	3.230	4.236	2.438	2.143	4.112
313.15	3.084	4.182	2.286	2.013	3.891
318.15	2.939	4.133	2.134	1.882	3.670
323.15	2.800	4.097	1.987	1.758	3.454
328.15	2.657	4.064	1.835	1.629	3.235

ΔG_a^{sp} (T) (in kJ/mol)			**R-K**		
T(K)	**CH_2Cl_2**	**$CHCl_3$**	**THF**	**Ethyl acetate**	**Acetone**
303.15	3.449	4.351	2.641	2.306	4.372
308.15	3.300	4.291	2.487	2.174	4.149
313.15	3.153	4.236	2.335	2.044	3.928
318.15	3.008	4.189	2.183	1.914	3.707
323.15	2.862	4.147	2.030	1.784	3.486

328.15	2.719	4.115	1.878	1.656	3.267

ΔG_a^{sp} (T) (in kJ/mol)			Geometric		
T(K)	**CH_2Cl_2**	**$CHCl_3$**	**THF**	**Ethyl acetate**	**Acetone**
303.15	4.712	3.114	0.155	2.306	1.769
308.15	4.480	2.890	0.079	2.210	1.644
313.15	4.249	2.666	0.004	2.114	1.519
318.15	4.018	2.443	-0.072	2.018	1.394
323.15	3.787	2.220	-0.147	1.922	1.269
328.15	3.557	1.998	-0.223	1.827	1.144

ΔG_a^{sp} (T) (in kJ/mol)			Spherical		
T(K)	**CH_2Cl_2**	**$CHCl_3$**	**THF**	**Ethyl acetate**	**Acetone**
303.15	4.294	4.309	2.502	3.216	5.463
308.15	4.134	4.317	2.346	3.040	5.190
313.15	3.974	4.330	2.189	2.865	4.918
318.15	3.817	4.350	2.034	2.692	4.648
323.15	3.660	4.379	1.880	2.521	4.379
328.15	3.505	4.417	1.725	2.351	4.111

ΔG_a^{sp} (T) (in kJ/mol)			Hamieh model		
T(K)	**CH_2Cl_2**	**$CHCl_3$**	**THF**	**Ethyl acetate**	**Acetone**
303.15	4.190	0.500	5.811445	6.94186	5.074
308.15	4.137	0.545	5.762945	6.86386	5.005
313.15	4.095	0.575	5.714445	6.78586	4.944
318.15	4.062	0.588	5.665945	6.70786	4.889
323.15	4.039	0.587	5.617445	6.62986	4.841
328.15	4.026	0.569	5.568945	6.55186	4.800

ΔG_a^{sp} (T) (in kJ/mol)			Boiling point		
T(K)	**CH_2Cl_2**	**$CHCl_3$**	**THF**	**Ethyl acetate**	**Acetone**
303.15	1.782	0.689	0.910	0.521	0.992
308.15	1.628	0.491	0.834	0.513	0.929
313.15	1.474	0.291	0.756	0.505	0.864
318.15	1.319	0.092	0.679	0.496	0.800
323.15	1.165	-0.107	0.602	0.488	0.735
328.15	1.010	-0.306	0.524	0.479	0.671

ΔG_a^{sp} (T) (in kJ/mol)			Vapor pressure		
T(K)	**CH_2Cl_2**	**$CHCl_3$**	**THF**	**Ethyl acetate**	**Acetone**
303.15	1.079	1.213	0.709	1.950	0.502

308.15	0.972	1.013	0.622	1.956	0.473
313.15	0.863	0.810	0.534	1.958	0.442
318.15	0.754	0.609	0.448	1.961	0.413
323.15	0.643	0.406	0.361	1.961	0.382
328.15	0.532	0.204	0.275	1.960	0.352

ΔG_a^{sp} (T) (in kJ/mol)	**Deformation polarizability**				
T(K)	**CH_2Cl_2**	**$CHCl_3$**	**THF**	**Ethyl acetate**	**Acetone**
303.15	-1.727	3.902	5.949	4.175	7.528
308.15	-1.819	3.645	5.781	4.100	7.346
313.15	-1.909	3.389	5.614	4.027	7.165
318.15	-1.999	3.133	5.446	3.953	6.984
323.15	-2.090	2.876	5.279	3.879	6.802
328.15	-2.181	2.620	5.111	3.805	6.621

ΔG_a^{sp} (T) (in kJ/mol)	**Topological index**				
T(K)	**CH_2Cl_2**	**$CHCl_3$**	**THF**	**Ethyl acetate**	**Acetone**
303.15	7.609	7.860	3.478	2.601	5.765
308.15	7.350	7.532	3.355	2.555	5.615
313.15	7.092	7.205	3.233	2.510	5.466
318.15	6.834	6.878	3.110	2.465	5.316
323.15	6.575	6.550	2.987	2.420	5.167
328.15	6.316	6.223	2.864	2.374	5.017

ΔG_a^{sp} (T) (in kJ/mol)	**DHvap**				
T(K)	**CH_2Cl_2**	**$CHCl_3$**	**THF**	**Ethyl acetate**	**Acetone**
303.15	-0.757	0.864	0.101	-0.649	-0.301
308.15	-0.865	0.662	0.038	-0.636	-0.342
313.15	-0.974	0.460	-0.024	-0.624	-0.382
318.15	-1.082	0.258	-0.086	-0.611	-0.423
323.15	-1.191	0.056	-0.149	-0.598	-0.464
328.15	-1.299	-0.146	-0.211	-0.585	-0.504

Table SI24. Values of the specific enthalpy ($-\Delta H_a^{sp}\ in\ kJ\ mol^{-1}$) of the various polar solvents adsorbed on UiO-66 surface by using vapor pressure, deformation polarizability and topological index methods compared to the various molecular models and global average.

Model or method	CH_2Cl_2	Chloroform	Ether	THF	Acetonitrile	Toluene	Benzene
Vapor pressure	7.317	5.893	28.191	21.262	22.724	3.609	3.174
Deformation polarizability	5.539	7.727	45.741	24.018	49.862	6.200	2.395
Topological index	16.072	13.155	33.863	21.753	40.644	6.600	2.395
Kiselev	18.395	17.889	27.537	57.460	14.866	9.905	3.500
Sphrical	11.698	9.831	35.462	35.462	47.097	5.003	4.512
Geometric	13.331	2.736	29.071	39.241	36.339	1.311	1.980
VDW	10.158	30.327	22.105	34.814	30.363	3.383	2.346
Redlich-Kwong	10.084	30.240	22.101	44.450	30.395	3.379	2.346
Cylindrical	14.708	21.070	18.580	54.630	37.971	7.919	3.120
Hamieh model	15.724	12.062	47.263	48.334	39.197	7.600	1.120
Global average	12.303	15.093	30.991	38.142	34.946	5.491	2.689

Table SI25. Values of the specific entropy ($-\Delta S_a^{sp} in\ J\ K^{-1} mol^{-1}$) of the various polar solvents adsorbed on UiO-66 catalyst by using vapor pressure, deformation polarizability and topological index methods compared to the various molecular models and global average.

Model or method	CH_2Cl_2	Chloroform	Ether	THF	Acetonitrile	Toluene	Benzene
Vapor pressure	8.1	9.4	32.3	36.5	42.4	5	0.3
Deformation polarizability	2.1	1.1	60.8	40.9	84.9	5.6	4.2
Topological index	11.9	7	39.9	37.6	68.4	2.1	1.2
Kiselev	23	22.6	32.8	64.3	30.3	20	2.1
Sphrical	10.6	9	49.8	49.8	93.2	11.5	11.2
Geometric	12.1	18.5	35.2	63	68.1	3.4	3.2
VDW	7.2	63.6	37.4	47.5	56.5	6.8	6.3
Redlich-Kwong	6.9	63	37.3	89.3	56.6	6.8	6.3
Cylindrical	14.2	33.1	29.7	75.3	72.3	13.9	3.5
Hamieh model	21.8	20.3	47.1	44.8	6.5	12.1	0.5
Global average	11.79	24.76	40.23	54.9	57.92	8.72	3.88

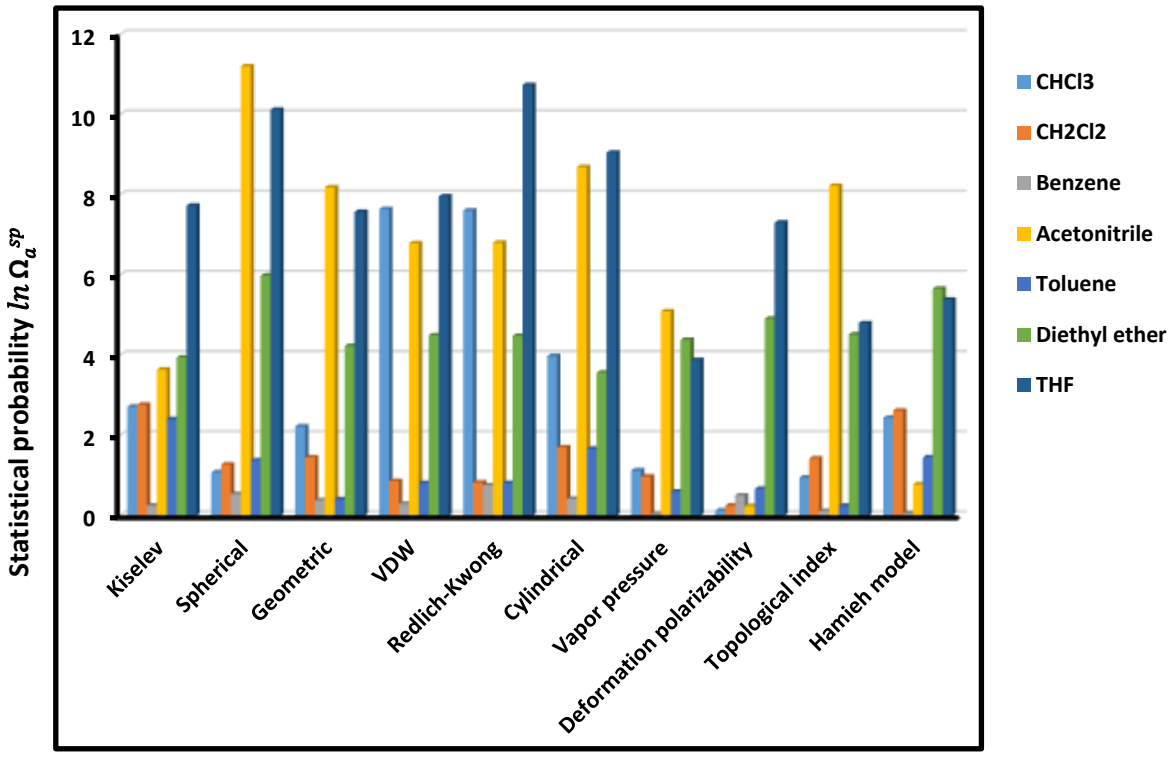

Figure SI 1. Values of the specific statistical probability of interaction of the various polar solvents adsorbed on the catalyst for the molecular models and methods.

List of abbreviations

a: the surface area of one adsorbed molecule,

a_{-CH2-}: the surface area of methylene group equal to 6 $Å^2$

a_n (T): surface area of n-alkane at a temperature T.

AN: acceptor number of electrons of probe

BET: Brunauer-Emmett-Teller

$C(T)$: constant depending on the reference state of adsorption

$C_nH_{2(n+1)}$: the general formula of n-alkanes

$-CH2-$: methylene group

D_c: the corrected flow rate

DCM: dichloromethane

D_m: the measured flow rate

DMF: N, N-dimethylformamide

DN: donor number of electrons of probe

H: the Planck's constant.

IGC: Inverse gas chromatography

J: a correction factor taking into account the compression of the gas

K: constant depending on the permittivity of the vacuum and the solid surface.

K_A: the acid constant of a solid

K_D: the base K_D constant of a solid

MOFs: metal-organic frameworks

n_C: the carbon atom number

$\mathcal{N}$: Avogadro's number,

P_0: the vapor pressure of the probe

PE: polyethylene

PTFE: polytetrafluoroethylene

PXRD: Powder X-ray Diffraction

R: the ideal gas constant,

SEM : Scanning Electron Microscopy

T: the absolute temperature

t_0: the zero retention reference time

T_a: the room temperature

T_c: the column temperature

TGA: Thermogravimetric Analysis

THF: tetrahydrofuran

t_R: the retention time of the probe

VDW: Van der Waals

Vn: the net retention volume

α, β: constants depending on the probe nature.

$\alpha_{0,s}$: the polarizability of molecule,

β_n: the surface area of n-alkanes at 0 K.

γ_{-CH2-}: the surface energy of methylene group

$\eta(T)$: the gas viscosity at temperature *T*,

γ_l^d: the dispersive component of the surface tension of the probe

γ_s^d: the dispersive component of the surface energy of a solid

χ_T: topological index of molecule

λ_n: the dilatation rate

ν_L: the electronic frequency of the probe

ν_s is the electronic frequency of the solid,

ω_A, ω_D: entropic acid and base parameters

$(-\Delta G^0)$: the free enthalpy of adsorption of the probe

ΔG_i^0: the standard free energy of component i

$(-\Delta G^d)$: the dispersive free enthalpy of adsorption

$(-\Delta G^{sp})$: the specific free enthalpy of adsorption

ΔH_a^0: differential heat of a probe

$(-\Delta H^{sp})$: the specific enthalpy

ΔS_a^0: entropy change of adsorption of a probe.

$(-\Delta S^{sp})$: the specific entropy

ΔP: the pressure change.

Ω_a^{sp}: the specific statistical probability of interaction